LETTER TO THE EDITOR

Recurrence relation for relativistic atomic matrix elements

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Abstract. Recurrence formulae for arbitrary hydrogenic radial matrix elements are obtained in the Dirac form of relativistic quantum mechanics. Our approach is inspired on the relativistic extension of the second hypervirial method that has been succesfully employed to deduce an analogous relationship in non relativistic quantum mechanics. We obtain first the relativistic extension of the second hypervirial and then the relativistic recurrence relation. Furthermore, we use such relation to deduce relativistic versions of the Pasternack-Sternheimer rule and of the virial theorem.

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For explaining certain features of atomic spectra, of atom-laser multiphoton transitions and of other atomic or molecular processes, a knowledge of matrix elements of polynomial radial functions between radial hydrogenic eigenstates is obviously of major importance (Moss 1972, Wong and Yeh 1983a, De Lange and Raab 1991, Quiney *et al* 1997). Such importance comes about since the r^λ terms can be regarded as explicit expressions for interatomic potentials or as terms in a multipolar description of the interaction with the electromagnetic field. In that area a great deal of work has been done in nonrelativistic quantum mechanics (Núñez-Yépez *et al* 1997, 1995 and the references therein). Nowadays, however, the sophisticated experimental techniques available make necessary the knowledge of such matrix elements between *relativistic* hydrogenic states. Though it is possible to compute directly such matrix elements (Kobus *et al* 1987, Wong and Yeh 1983b) the computations quickly become cumbersome thus techniques for evaluating any number of them starting from a few known ones are extremely convenient. For example, motivated by the need of evaluating the curvature-induced modifications of the hydrogen spectrum Bessis *et al* (1985) have contributed in this direction. In spite of this, however, there is not as yet any valid recurrence relation in relativistic quantum mechanics analogous to the general and useful ones customarily used in ordinary quantum mechanics.

In this work we derive one such recurrence relation between relativistic radial hydrogenic states; this relation expresses the matrix elements of r^λ and βr^λ (where β is the Dirac matrix) in terms of those of $r^{\lambda-1}$, $\beta r^{\lambda-1}$, $r^{\lambda-2}$, $\beta r^{\lambda-2}$, $r^{\lambda-3}$, and $\beta r^{\lambda-3}$—as given in equations (17) and (20) below. The recurrence relations we obtain here can be regarded as a generalization of the non relativistic Blanchard rule (Núñez-Yépez *et al* 1995, Blanchard 1974) to the bound hydrogenic radial eigenstates of Dirac relativistic quantum mechanics. Such relation can be found useful in, for example, different schemes of perturbation theory used in atomic calculations (Brack 1983, Dobrovolska and Tutik 1999) or for computing the effect of external fields on bound electrons (Wong and Yeh 1983a, b). Please be aware that we only intend to give the main results in this communication, for most of the details and other possible applications see Martínez-y-Romero *et al* (2000).

The Dirac Hamiltonian, the Dirac equation for the stationary states of the hydrogen atom, and the corresponding energy eigenvalues, are

$$H_D = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 - \frac{Z\alpha_F\hbar c}{r}, \quad H_D\,\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r}),$$
$$E = mc^2\left(1 + \frac{Z^2\alpha_F^2}{\left(n - j - 1/2 + \sqrt{(j+1/2)^2 - Z^2\alpha_F^2}\right)^2}\right)^{-1/2} \tag{1}$$

where $\boldsymbol{\alpha}$ and β are standard 4×4 Dirac matrices in the Dirac representation (Bjorken and Drell 1964; Drake 1996, Ch 22 by Grant I P), Z is the atomic number, r

the relative distance between the electron and the nucleus, m the electron mass, c the speed of ligth, $\alpha_F \equiv e^2/4\pi\epsilon_0\hbar c$ the fine structure constant, e the electron charge, $j = 1/2, 3/2, 5/2, \ldots$ the total angular momentum quantum number, and $n = 0, 1, 2, \ldots$ is the principal quantum number. The obvious rotational symmetry of H_D implies that the bound eigenstates of the hydrogen atom can be written as

$$\Psi_{n,\kappa,m_z}(r,\theta,\phi) = \frac{1}{r}\begin{pmatrix} F_{n,j,\epsilon}(r)\chi_{\kappa,m_z}(\theta,\phi) \\ \\ \mathrm{i}G_{n,j,\epsilon}(r)\chi_{-\kappa,m_z}(\theta,\phi) \end{pmatrix}. \tag{2}$$

where $m_z = -j, -j+1/2, \ldots, j-1/2, j$, is the z-projection of the total angular momentum quantum number, and $\chi_{\kappa,m_z}(\theta,\phi)$ and $\chi_{-\kappa,m_z}(\theta,\phi)$ are spinor spherical harmonics of opposite parity and $\kappa = -\epsilon(j+1/2)$ is the eigenvalue of the operator $\Lambda \equiv \beta(1 + \boldsymbol{\Sigma}\cdot\mathbf{L})$ ($\boldsymbol{\Sigma} \equiv \boldsymbol{\sigma}\otimes I = \mathrm{diag}(\boldsymbol{\sigma},\boldsymbol{\sigma})$, $\boldsymbol{\sigma}$ is the vector with Pauli matrices as components), which can be seen to commute with H_D (Drake 1996, Ch 22 by Grant I P). We found it convenient to define the quantum number $\epsilon = (-1)^{j+l-1/2}$— *i.e.* ϵ equals $+1$ when $l = j+1/2$ or equals -1 when $l = j-1/2$— and use it instead of parity for labeling the eigenstates, so $l = j + \epsilon/2$ and $l' = j - \epsilon/2$, because the small component has the opposite parity to the big one (Martínez-y-Romero *et al* 1998, 1999). Please notice that another notation for the spinor functions used in (2) is $\mathcal{Y}^{l}_{j,m_z} \equiv \chi_{\kappa,m_z}$ and $\mathcal{Y}^{l'}_{j,m_z} \equiv \chi_{-\kappa,m_z}$ (Martínez-y-Romero *et al* 1998, Greiner 1991, Moss 1972). Writing the eigenfunctions in the form (2) completely solves the angular part of the problem, so we only need to cope with the radial part of it. Be aware also that, as we did in (2), we prefer to employ n, j and ϵ rather than just n, and κ to label the radial eigenfunctions.

Let us begin establishing a relativistic version of the hypervirial result which is known to lead directly—though not straightforwardly because the computations are rather long— to the Blanchard recurrence relation in nonrelativistic quantum mechanics (Núñez-Yépez *et al* 1995). The radial Hamiltonian associated to (1) can be obtained using the squared total (orbital plus spin) angular momentum $\mathbf{J}^2 = \mathbf{L}^2 + \boldsymbol{\sigma}\cdot\mathbf{L} + 3/4$, and the fact that the operator $\mathbf{L}^2$, as applied on eigenstates of the form (2), is equivalent to the action of the operator $j(j+1) + \epsilon\beta(j+1/2) + 1/4$ upon the same states. Thus, using $(\boldsymbol{\alpha}\cdot\mathbf{r})(\boldsymbol{\alpha}\cdot\mathbf{p}) = (\boldsymbol{\Sigma}\cdot\mathbf{r})(\boldsymbol{\Sigma}\cdot\mathbf{p}) = \mathbf{r}\cdot\mathbf{p} + \mathrm{i}\boldsymbol{\Sigma}\cdot\mathbf{L}$, we get $\boldsymbol{\alpha}\cdot\mathbf{p} = \alpha_r\left[p_r - i\beta(j_k+1/2)\epsilon_k/r\right]$, so we finally obtain (Martínez-y-Romero *et al* 2000)

$$\begin{aligned} H_k &= \alpha_r\left[p_r - i\beta\frac{\epsilon_k}{r}\left(j_k + \frac{1}{2}\right)\right] + \beta m + V(r), \\ \\ H_k\psi_k(r) &= E_k\psi_k(r), \end{aligned} \tag{3}$$

where we use units such that $\hbar = c = 1$, $V(r)$ is an arbitrary radial potential, k is a label introduced for the sake of later convenience, and

$$\alpha_r = \boldsymbol{\alpha}\cdot\frac{\mathbf{r}}{r} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \qquad p_r = -\frac{\mathrm{i}}{r}\frac{d}{dr}\,r,$$
$$\psi_k(r) \equiv \psi_{n_k,j_k,\epsilon_k}(r) = \frac{1}{r}\begin{pmatrix} F_{n_k,j_k,\epsilon_k}(r) \\ \mathrm{i}G_{n_k,j_k,\epsilon_k}(r) \end{pmatrix}. \tag{4}$$

As it should be clear from the matrix expression for α_r in the previous equation, we can use a 2×2 representation valid for the radial eigenstates given in (4)—where the now 2×2 β-matrix is just diag$(1,-1)$ with numerical entries (Constantinescu and Magyari 1971, p 382). Using this representation the purely radial Dirac equation reduces to

$$\begin{bmatrix} m+(V(r)-E) & Z\epsilon(j+1/2)/r - d/dr \\ Z\epsilon(j+1/2)/r + d/dr & m-(V(r)-E) \end{bmatrix}\begin{bmatrix} F_{nj\epsilon}(r) \\ G_{nj\epsilon}(r) \end{bmatrix} = 0; \tag{5}$$

we have to point out, however, that using this representation is not strictly necessary and that all our results are representation independent.

The key relationship needed for deriving the relativistic recurrence relation stems directly from equation (3)—compare with equation (2) and the nonrelativistic discussion that follows in (Núñez-Yépez *et al* 1995 pp. L526–L527).

Let us first compute matrix elements of the radial function $\xi(r) \equiv H_2 f(r) - f(r)H_1$ between radial eigenstates of the hydrogen atom in the energy basis, where $f(r)$ is an arbitrary radial function and the H_i are the radial Hamiltonians appearing in (3). Evaluating such radial matrix elements we get

$$\begin{aligned}(E_2-E_1)&\langle n_2\, j_2\, \epsilon_2|f(r)|n_1\, j_1\, \epsilon_1\rangle \\ &= \langle n_2\, j_2\, \epsilon_2|H_2 f(r) - f(r)H_1|n_1\, j_1\, \epsilon_1\rangle \\ &= -\mathrm{i}\langle n_2\, j_2\, \epsilon_2|\alpha_r\left(f'(r) + \frac{\Delta_{21}^-}{2r}\beta f(r)\right)|n_1\, j_1\, \epsilon_1\rangle, \end{aligned} \tag{6}$$

where $\quad |n\, j\, \epsilon\rangle \equiv \begin{pmatrix} F_{nj\epsilon} \\ \mathrm{i}G_{nj\epsilon} \end{pmatrix},$

we have defined the quantities $\Delta_{21}^{\pm} \equiv \epsilon_2(2j_2+1) \pm \epsilon_1(2j_1+1)$, and the expressions used for the $\langle n_2\, j_2\, \epsilon_2|f(r)|n_1\, j_1\, \epsilon_1\rangle$ and the $\langle n_2\, j_2\, \epsilon_2|\beta f(r)|n_1\, j_1\, \epsilon_1\rangle$ matrix elements are

$$\begin{aligned}\langle n_2 j_2 \epsilon_2|f(r)|n_1 j_1 \epsilon_1\rangle &= \int f(r)\left[F_1(r)F_2^*(r) + G_1(r)G_2^*(r)\right]dr, \\ \langle n_2 j_2 \epsilon_2|\beta f(r)|n_1 j_1 \epsilon_1\rangle &= \int f(r)\left[F_1(r)F_2^*(r) - G_1(r)G_2^*(r)\right]dr. \end{aligned} \tag{7}$$

We then apply the result (6) to the function $H_2\xi(r) - \xi(r)H_1$, to obtain

$$\begin{aligned}
&(E_2 - E_1)^2\langle s_2|f(r)|s_1\rangle = \\
&\langle s_2| - \frac{\Delta_{21}^-}{2r^2}\beta f(r) - f''(r) - \frac{\Delta_{21}^-}{2r}f'(r)\beta - \frac{\Delta_{21}^-}{r}f(r)\beta\frac{d}{dr} + \\
&\frac{\Delta_{21}^+}{2r}f'(r)\beta + \left(\frac{\Delta_{21}^-}{2r}\right)^2 f(r) + 2\mathrm{i}\alpha_r\beta m\left(f'(r) + \frac{\Delta_{21}^-}{2r}\beta f(r)\right)|s_1\rangle;
\end{aligned} \tag{8}$$

where the subscripts in the radial components, F and G, stand for the three quantum numbers n, j, ϵ, and we have assumed $\Delta_{21}^- \neq 0$. From now on, as we did in equation (8), we use the *shorthand* $|s_i\rangle \equiv |n_i\, j_i\, \epsilon_i\rangle$ for the states of the system. It is to be noted that (8) can be regarded as the relativistic equivalent to the hypervirial obtained in (Núñez-Yépez *et al* 1995, equation (8), p. L526).

However, in the Dirac case we are dealing with, at difference to what happens in the nonrelativistic case, equation (8) is not enough for deriving the recurrence relation between matrix elements of powers of r, we also need the following results (Martínez-y-Romero *et al* 2000):
a) A second order iteration for certain non diagonal matrix elements, where we use for computing the elements, the radial function $H_2\xi(r) + \xi(r)H_1$

$$\begin{aligned}
&(E_2^2 - E_1^2)\langle s_2|f(r)|s_1\rangle = \langle s_2|H_2\xi + \xi H_1|s_1\rangle = \\
&\langle s_2| - \frac{2f'(r)}{r} + \frac{\Delta_{21}^-}{2r^2}\beta f(r) - f''(r) - 2f'(r)\frac{d}{dr} + \\
&\frac{\Delta_{21}^+\Delta_{21}^-}{4r^2}f(r) - 2\mathrm{i}\alpha_r\left(f'(r) + \frac{\Delta_{21}^-}{2r}\beta f(r)\right)V(r)|s_1\rangle,
\end{aligned} \tag{9}$$

b) the following matrix elements

$$\begin{aligned}
-\mathrm{i}(E_2 + E_1)\langle s_2|\alpha_r f(r)|s_1\rangle = -\langle s_2|&\frac{2f(r)}{r} + f'(r) + 2f(r)\frac{d}{dr} \\
&-\frac{\Delta_{21}^-}{2r}\beta f(r) + 2\mathrm{i}\alpha_r V(r)f(r)|s_1\rangle,
\end{aligned} \tag{10}$$

c) the matrix elements of the radial function $-\mathrm{i}(H_2\alpha_r f(r) - \alpha_r f(r)H_1)$, lead to

$$\begin{aligned}
&-\mathrm{i}(E_2 - E_1)\langle s_2|\alpha_r f(r)|s_1\rangle = \\
&\qquad\langle s_2| - f'(r) + \frac{\Delta_{21}^+}{2r}\beta f(r) + 2\mathrm{i}\alpha_r\beta m f(r)|s_1\rangle.
\end{aligned} \tag{11}$$

and, d) the matrix elements of the radial function $H_2\beta f(r) + \beta f(r)H_1$, lead to (Martínez-y-Romero 2000)

$$(E_2+E_1)\langle s_2|\beta f(r)|s_1\rangle = \langle s_2|\mathrm{i}\beta\alpha_r f'(r) - \mathrm{i}\alpha_r\frac{\Delta_{21}^-}{2r}f(r) + 2\left[m+\beta V(r)\right]f(r)|s_1\rangle. \tag{12}$$

Equations (6) and (8–12) are the basic equations for our problem. For more details on the computations please see Martínez-y-Romero *et al* (2000).

Up to this point, our results are valid both for an arbitrary radial potential $V(r)$ and for an arbitrary radial function $f(r)$ but, to be specific, let us assume that $V(r)$ is precisely the Coulomb potential, *i.e.*

$$V(r) = -\frac{Z}{r}, \tag{13}$$

where we have taken $e^2/4\pi\epsilon_0 = 1$. In this work we consider only the case of functions of the form $f(r) = r^\lambda$; so, putting $f(r) = r^{\lambda-1}$ in equation (6) and in equation (10), extracting the term with $-\mathrm{i}\alpha_r\Delta_{21}^-\beta r^{\lambda-2}$ from the former and the term with $-2\lambda r^{\lambda-1}d/dr$ from the latter and substituting them into equation (9), but evaluated using $f(r) = r^\lambda$, we get

$$\begin{aligned}(E_2^2-E_1^2)\langle s_2|r^\lambda|s_1\rangle = \langle s_2|\frac{\Delta_{21}^-\Delta_{21}^+}{4}r^{\lambda-2} + \frac{\Delta_{21}^-}{2}(1-\lambda)\beta r^{\lambda-2} + \\ Z\left[2\mathrm{i}\alpha_r r^{\lambda-2}(1-\lambda) - 2(E_2-E_1)r^{\lambda-1}\right] - (E_2+E_1)\lambda\mathrm{i}\alpha_r r^{\lambda-1}|s_1\rangle.\end{aligned} \tag{14}$$

We next use $f(r) = r^\lambda$ in equation (6), extract the term with $2\mathrm{i}\alpha_r\beta m r^{\lambda-1}$ and substitute it into (11) but evaluated using $f(r) = r^{\lambda-1}$, to obtain the following result

$$\begin{aligned}\left[(E_2-E_1) - \frac{4m\lambda}{\Delta_{21}^-}\right]\langle s_2|(-\mathrm{i}\alpha_r r^{\lambda-1})|s_1\rangle = \\ \langle s_2| - (\lambda-1)r^{\lambda-2} - \frac{4m}{\Delta_{21}^-}(E_2-E_1)r^\lambda + \frac{\Delta_{21}^+}{2}\beta r^{\lambda-2}|s_1\rangle;\end{aligned} \tag{15}$$

then, we use $f(r) = r^\lambda$ in equation (12) and follow the same procedure as above, to get instead

$$\begin{aligned}\left[(E_2-E_1) - \frac{\Delta_{21}^- m}{\lambda}\right]\langle s_2|(-\mathrm{i}\alpha_r r^{\lambda-1})|s_1\rangle = \langle s_2| - (\lambda-1)r^{\lambda-2} + \\ \frac{4m^2}{\lambda}r^\lambda + \frac{\Delta_{21}^+}{2}\beta r^{\lambda-2} - \frac{4Zm}{\lambda}\beta r^{\lambda-1} - \frac{2m}{\lambda}(E_2+E_1)\beta r^\lambda|s_1\rangle.\end{aligned} \tag{16}$$

To continue, we evaluate equation (15) first using $f(r) = r^{\lambda-1}$ and then using $r^{\lambda-2}$, next we extract the term $-\mathrm{i}\alpha_r\lambda(E_2+E_1)r^{\lambda-1}$ from the former and the term

$-2\mathrm{i}Z\alpha_r(\lambda-1)r^{\lambda-2}$ from the latter, to finally obtain, on substituting these extracted terms into (14), the recurrence relation

$$c_0\langle s_2|r^{\lambda}|s_1\rangle=\sum_{i=1}^{3}c_i\langle s_2|r^{\lambda-i}|s_1\rangle+\sum_{i=2}^{3}d_i\langle s_2|\beta r^{\lambda-i}|s_1\rangle, \tag{17}$$

where the numbers c_i, $i=0,\ldots 3$ are given by

$$\begin{aligned}
c_0&=\frac{(E_2^2-E_1^2)(E_2-E_1)\Delta_{21}^{-}}{(E_2-E_1)\Delta_{21}^{-}-4m\lambda},\\
c_1&=-\frac{2Z(E_2-E_1)^2\Delta_{21}^{-}}{(E_2-E_1)\Delta_{21}^{-}-4m(\lambda-1)},\\
c_2&=\frac{\Delta_{21}^{-}\Delta_{21}^{+}}{4}-\lambda(\lambda-1)\frac{(E_1+E_2)\Delta_{21}^{-}}{(E_2-E_1)\Delta_{21}^{-}-4m\lambda},\\
c_3&=\frac{-2Z(\lambda-1)(\lambda-2)\Delta_{21}^{-}}{(E_2-E_1)\Delta_{21}^{-}-4m(\lambda-1)},
\end{aligned} \tag{18}$$

and the numbers d_i, $i=2$ and 3, by

$$\begin{aligned}
d_2&=\frac{\Delta_{21}^{-}}{2}\left[(1-\lambda)+\frac{\lambda(E_2+E_1)\Delta_{21}^{+}}{(E_2-E_1)\Delta_{21}^{-}-4m\lambda}\right],\\
d_3&=\frac{Z(\lambda-1)\Delta_{21}^{-}\Delta_{21}^{+}}{(E_2-E_1)\Delta_{21}^{-}-4m(\lambda-1)}.
\end{aligned} \tag{19}$$

Equation (17), together with the specific values for the c_a and the d_a, can be regarded as the direct relativistic version of the Blanchard (1974) relation —compare with equations (10) and (11) in Núñez-Yépez *et al* (1995). These relations are valid inasmuch as the number $w_1+w_2+\lambda+1$ is greater than zero, where $w_i\equiv\sqrt{(j_i+1/2)^2-Z^2\alpha_F^2}=\sqrt{\kappa_i^2-Z^2\alpha_F^2}$. This condition amounts basically to the requirement that any integrand should be at least of the form $1/r^{1+\gamma}$ with $\gamma>0$ (Martínez-y-Romero *et al* 2000).

The extra complication in the recurrence relation (17), that does not occur in the nonrelativistic case, is the explicit appearance of matrix elements of powers of r times the β matrix. In a way, this is just a matter of a sign change in an integral—as it should be obvious from equation (7). However, since it is not possible to avoid the β dependence in (17), as it stands such equation does not really allow the computation of $\langle s_2|r^{\lambda}|s_1\rangle$ in terms of the $\langle s_2|r^{\lambda-i}|s_1\rangle$ $i=1,2,3$ as it undeniably happens in nonrelativistic quantum mechanics (Núñez-Yépez *et al* 1995), something additional is needed.

For obtaining the extra information required, we only need to multiply equation (16) times $(E_2-E_1)-4m\lambda/\Delta_{21}^{-}$ and equation (15) times $(E_2-E_1)-m\Delta_{21}^{-}/\lambda$, and then

substract the results, to finally obtain the lacking recurrence relation for the matrix elements involving the β matrix times r-powers, namely

$$\begin{aligned} e_0\langle s_2|\beta r^\lambda|s_1\rangle =& b_0\langle s_2|r^\lambda|s_1\rangle + b_2\langle s_2|r^{\lambda-2}|s_1\rangle + e_1\langle s_2|\beta r^{\lambda-1}|s_1\rangle \\ &+ e_2\langle s_2|\beta r^{\lambda-2}|s_1\rangle, \end{aligned} \tag{20}$$

where the numbers d_i and e_i $i = 1, 2, 3$ are given by

$$\begin{aligned} b_0 =& 4\lambda\left[(E_2 - E_1)^2 - 4m^2\right], \\ b_2 =& (1-\lambda)\left[(\Delta_{21}^-)^2 - 4\lambda^2\right], \\ e_0 =& 2(E_2 + E_1)[(E_2 - E_1)\Delta_{21}^- - 4m\lambda], \\ e_1 =& 4Z[4m\lambda - (E_2 - E_1)\Delta_{21}^-], \\ e_2 =& \frac{\Delta_{21}^+}{2}[(\Delta_{21}^-)^2 - 4\lambda^2]. \end{aligned} \tag{21}$$

The validity conditions of this recurrence relation is that the number $(w_1 + w_2 + \lambda + 1)$ be greater than zero, exactly as before.

Equations (17) and (20) are together the useful recurrence relations for evaluating radial matrix elements between relativistic radial hydrogenic states; in this sense they are thus the actual relativistic generalization of Blanchard rule.

The recurrence relation obtained above (17) pressupose $\Delta_{21}^- \neq 0$, but, for studying the diagonal case, we must have $\epsilon_1 = \epsilon_2$ and $j_1 = j_2$ (in other words $\kappa_1 = \kappa_2$) which precisely imply that $\Delta_{21}^- = 0$. In such instance we cannot apply that relation, we have to rederive the recurrence relation using as starting equations

$$(E_2 - E_1)\langle n_1\, j\, \epsilon|f(r)|n_2\, j\, \epsilon\rangle = \langle n_1\, j\, \epsilon|(-\mathrm{i}\alpha_r f'(r))|n_2\, j\, \epsilon\rangle, \tag{22}$$

$$\begin{aligned} (E_2 - E_1)\langle n_1\, j\, \epsilon| - \mathrm{i}\alpha_r f(r)|n_2\, j\, \epsilon\rangle =& \langle n_1\, j\, \epsilon| - f'(r) + \frac{\Delta^+}{2r}\beta f(r) + \\ &+ 2i\alpha_r\beta m f(r)|n_2\, j\, \epsilon\rangle, \end{aligned} \tag{23}$$

and

$$\begin{aligned} (E_2 + E_1)\langle n_1\, j\, \epsilon|\beta f(r)|n_2\, j\, \epsilon\rangle =& \langle n_1\, j\, \epsilon| - \mathrm{i}\alpha_r\beta f'(r) \\ &+ 2\left(m + \beta V(r)\right) f(r)|n_2\, j\, \epsilon\rangle, \end{aligned} \tag{24}$$

where, for avoiding possible misunderstandings, we have reverted to explicitly writing the quantum numbers in the states and $\Delta^+ \equiv 2\epsilon(2j+1)$. To get the result we want, we evaluate equation (22) with $f(r) = r^\lambda$, then we put $f(r) = r^{\lambda-1}$ in equation (23),

and $f(r) = r^{\lambda}$ in equation (24); thence, using essentially a procedure similar to the used in the $\Delta_{21}^{-} \neq 0$ case outlined above, we finally obtain (Martínez-y-Romero *et al* 2000)

$$\begin{aligned}\left[(E_2 - E_1)^2 - 4m^2\right] \langle n_1\, j\, \epsilon|r^{\lambda}|n_2\, j\, \epsilon\rangle &= \lambda\frac{\Delta_{21}^{+}}{2}\langle n_1\, j\, \epsilon|\beta r^{\lambda-2}|n_2\, j\, \epsilon\rangle \\ &- 4m\langle n_1\, j\, \epsilon|\beta r^{\lambda-1}|n_2\, j\, \epsilon\rangle - 2m(E_2 + E_1)\langle n_1\, j\, \epsilon|\beta r^{\lambda}|n_2\, j\, \epsilon\rangle \\ &- \lambda(\lambda-1)\langle n_1\, j\, \epsilon|r^{\lambda-2}|n_2\, j\, \epsilon\rangle.\end{aligned} \tag{25}$$

This is the version of the recurrence relation (17) which is valid when $\Delta_{21}^{-} = 0$. On the other hand, relation (20) can be directly written in the case $\Delta_{21}^{-} = 0$, giving a equation entirely equivalent to (25); so, in the case where $\Delta_{21} = 0$, we have relation (25) and relation (20) with the restriction $\Delta_{21} = 0$.

As happens with the non relativistic recurrence relation (Núñez-Yépez *et al* 1995), various of its particular cases have interest on their own; for example when $\lambda = 0$, from (25) we directly obtain

$$\begin{aligned}\left[(E_2 - E_1)^2 - 4m^2\right] \delta_{n_1 n_2} &= -4m\,\langle n_1\, j\, \epsilon|\frac{\beta}{r}|n_2\, j\, \epsilon\rangle \\ &- 2m\,(E_2 + E_1)\,\langle n_1\, j\, \epsilon|\beta|n_2\, j\, \epsilon\rangle,\end{aligned} \tag{26}$$

where δ_{ij} is a Kronecker delta. This relation (26) could be regarded as a relativistic version of the well-known Pasternak-Sternheimer (1962) rule of non relativistic quantum mechanics, which says that the expectation value between hydrogenic states of the $1/r^2$ potential, vanishes when the orbital angular momenta of the states 1 and 2 coincide, *i.e.* when $l_1 = l_2$. We remark that in the relativistic case the expectation value of the $1/r$ potential (which corresponds to the square root of $1/r^2$) times β, does **not** necessarily vanish even when the total angular momenta of the two states coincide: $j_1 = j_2$. This agrees with the known non relativistic fact that the Pasternack-Sternheimer rule is applicable to eigenfunctions of potentials whose energy eigenvalues depend only on the principal quantum number—which is not the case for the hydrogen atom in Dirac relativistic quantum mechanics.

Furthermore, in the completely diagonal case (*i.e.* when $n_1 = n_2$, $j_1 = j_2$, and $\epsilon_1 = \epsilon_2$; or just $n_1 = n_2$ and $\kappa_1 = \kappa_2$) we easily find ($\langle O\rangle$ stand for O's expectation value)

$$m = -\,\langle\beta V(r)\rangle + E\,\langle\beta\rangle = Z\left\langle\frac{\beta}{r}\right\rangle + E\,\langle\beta\rangle\,, \tag{27}$$

or, using $\langle\beta\rangle = E/m$ (De Lange and Raab 1991),

$$E^2 = m\,\langle\beta V(r)\rangle + m^2 = -m\,Z\left\langle\frac{\beta}{r}\right\rangle + m^2. \tag{28}$$

This last expression can be regarded as another version of the relativistic virial theorem in a form different from the one proposed by Kim (1967). Please notice that the first equalities in equations (27) and (28) above are valid for an arbitrary central potential $V(r)$.

Some other useful things that can be obtained from both the relativistic hypervirial [equation (8)] and the subsequent results [equations (9–12)], and from the relativistic recurrence relation presented in this contribution [equations (17) and (20)]; but such discussions as well as the many details left out from our presentation, will appear in a more detailed article (Martínez-y-Romero *et al* 2000). Let us pinpoint again that for our results to have meaning we need that the exponent in the recurrence relations, λ, comply with $(\lambda+1) > -w_1 - w_2$, where we assume that the $w_i = \sqrt{(j_i+1/2)^2 - Z^2\alpha_F^2}$ are real numbers (Martínez-y-Romero *et al* 2000). This condition has a similar form to the one required by Blanchard (1974) in the non relativistic case.

We have just learnt of the plans to test CPT and Lorentz invariance studying the 1s-2s two photon transition in hydrogen, in which the recurrence relations proposed here can be of some help for the computations (Bluhm *et al* 2000).

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